Development of the AMUSE Code

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Advanced Nuclear Fuel Cycle Initiative
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Purpose of AMUSE

AFCI

- The UREX+ process is being developed as part of the Advanced Aqueous Process Separations
- ANL work is centered on process design, modeling, and demonstration
- **The AMUSE code forms the computational basis for flowsheet design and process development**

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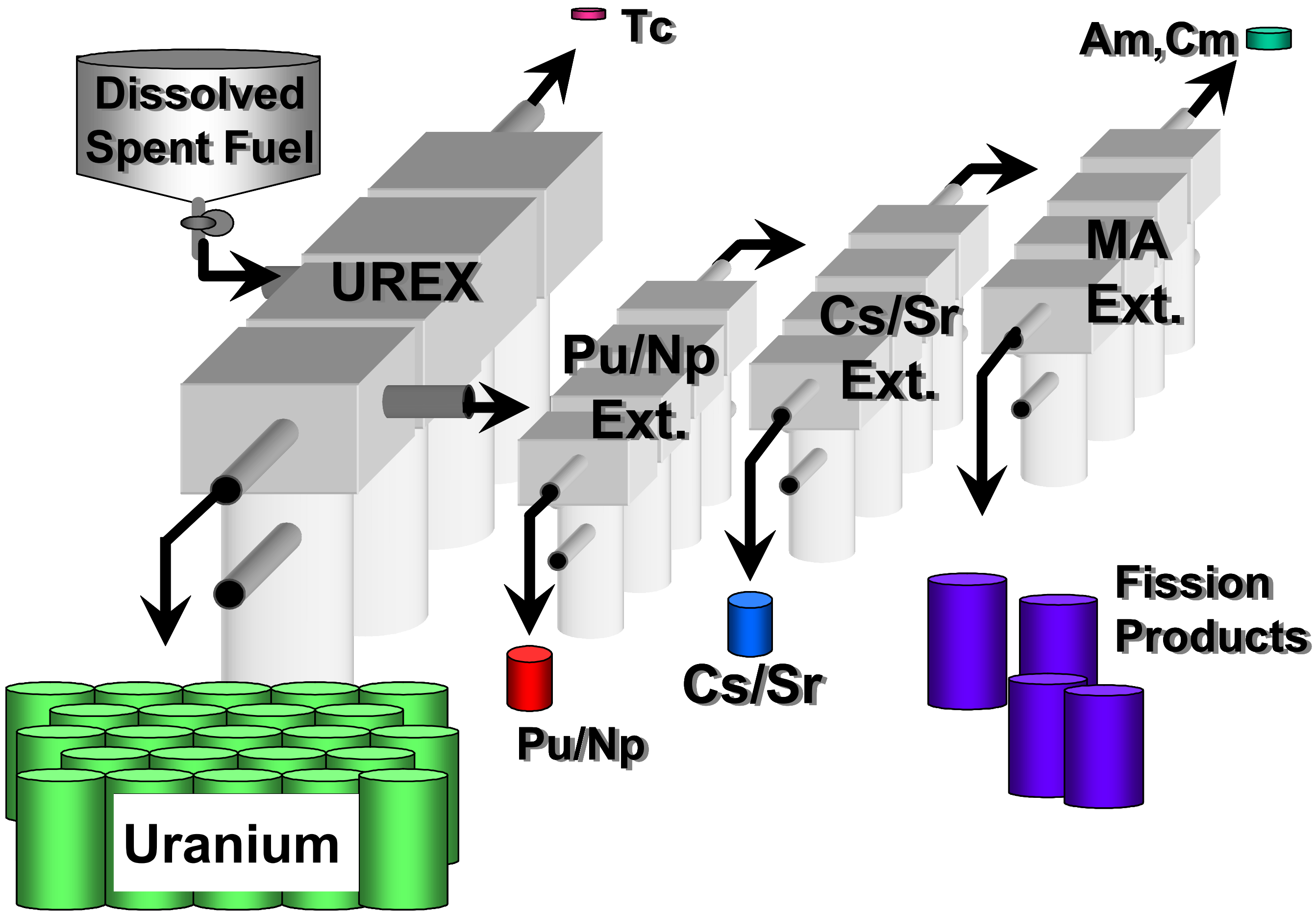
Advanced Aqueous Process Development – UREX+



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2003 Milestones

- Demonstrate UREX+ with spent fuel at ANL
  - Process includes U, Tc, Pu/Np, Cs/Sr, and Am/Cm separations
- Update Model
  - Add Pu/Np, Cs/Sr, and Am/Cm extraction processes to AMUSE
- Design, with other participants, flowsheet for UREX+ engineering scale demonstration at INEEL

UREX Flowsheets Design

- AMUSE was used to design countercurrent uranium solvent-extraction process demonstrations using
  - Simulated feed in FY 01 at ANL
  - Dissolved commercial fuel in FY 02 at SRTC

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Development of AMUSE

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Basis of AMUSE

- The Generic TRUEX Model (GTM) was developed in the 1980s to calculate flowsheets for treating High-Level Liquid Waste
- The keys to its success were
  - Developing algorithms from a firm understanding of the chemistry
  - Basing D values on chemically significant equilibria
    - i.e., not just fitting experimental data to power series
  - Using thermodynamic activities for hydrogen ion, nitrate, and water to fit experimental data to equilibrium equations
  - Building the model in a modular format with the easily programmed and user-friendly Microsoft Excel

The AMUSE Code

- The GTM was expanded to include UREX and PUREX processes
  - It is reborn as the **A**rgonne **M**odel for **U**niversal **S**olvent **E**xtraction (**AMUSE**)
- New front end was added for easier input
  - Currently using Visual Basic for Excel
  - Graphical user interface being developed in partnership with UNLV

AMUSE Capabilities

- Models for Solvent Extraction
  - TRUEX, SREX, UREX and PUREX
- Applications
  - Design flowsheet to meet specific process goals
  - Optimize flowsheet for robust performance
    - Variation in feed compositions
    - Variation in feed flow rates
  - Measure effects of process deviations caused by operational upsets or product diversion

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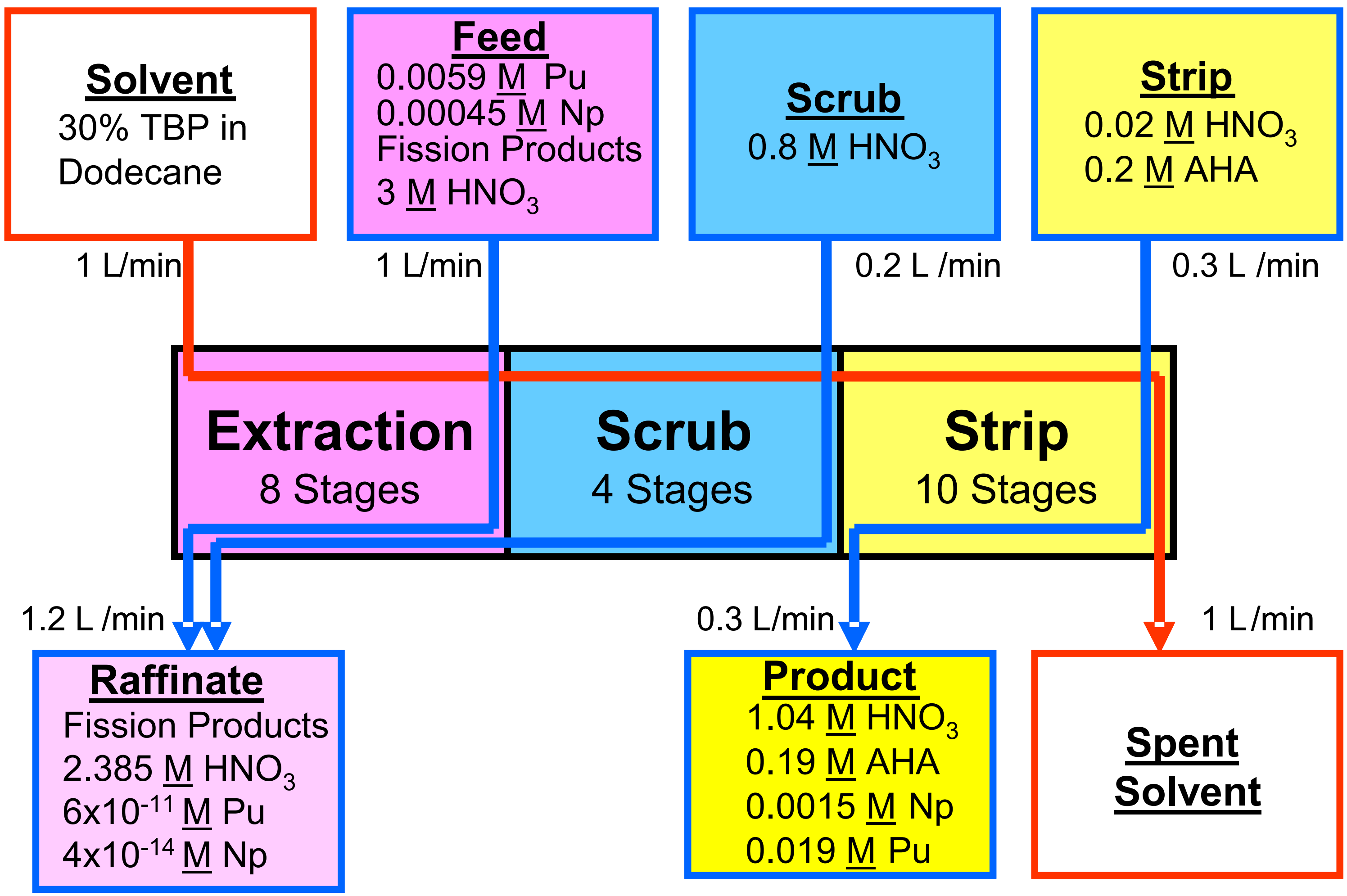
AMUSE Simulation

Pu/Np Separation from Fission Products



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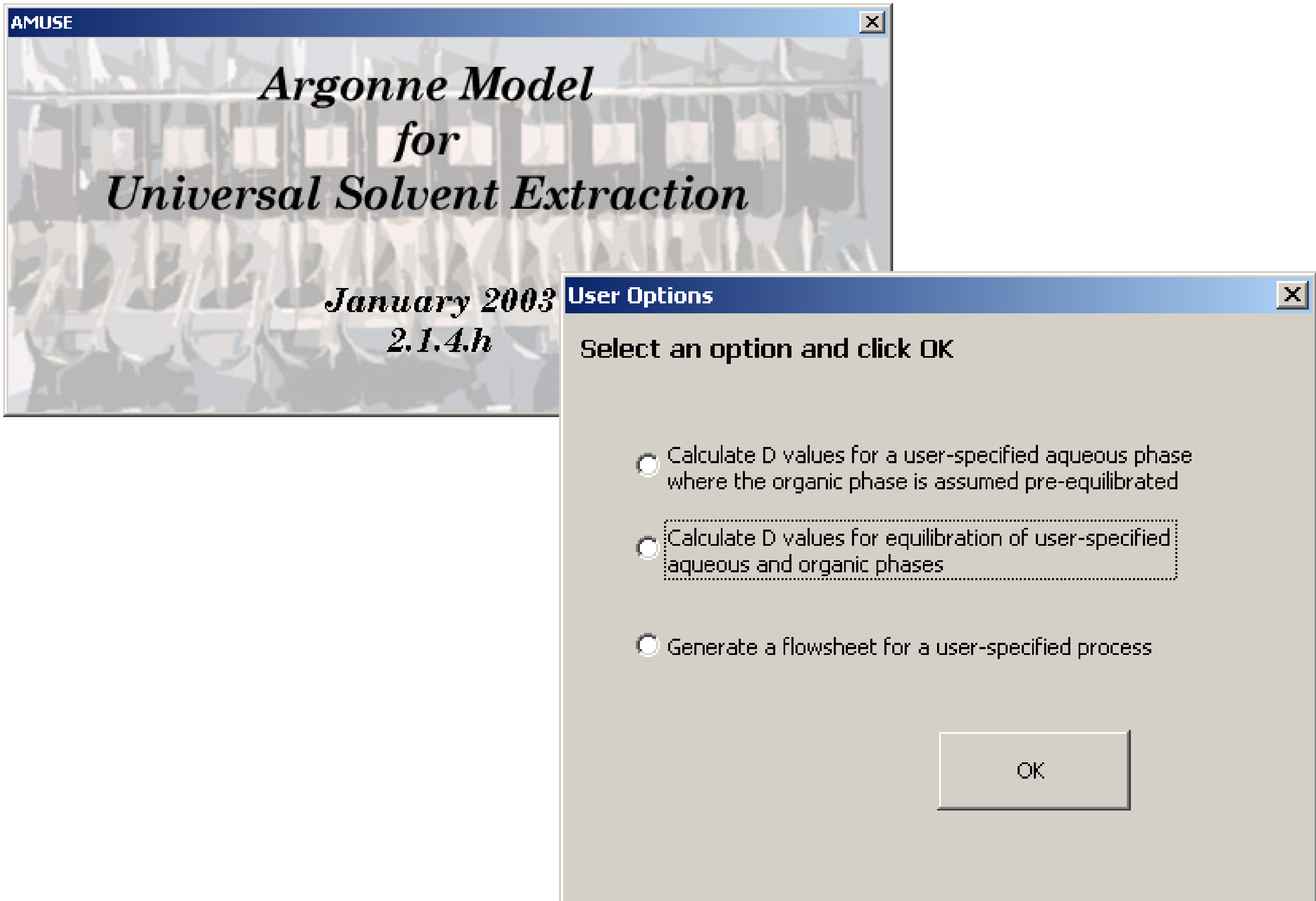
AMUSE Start-up



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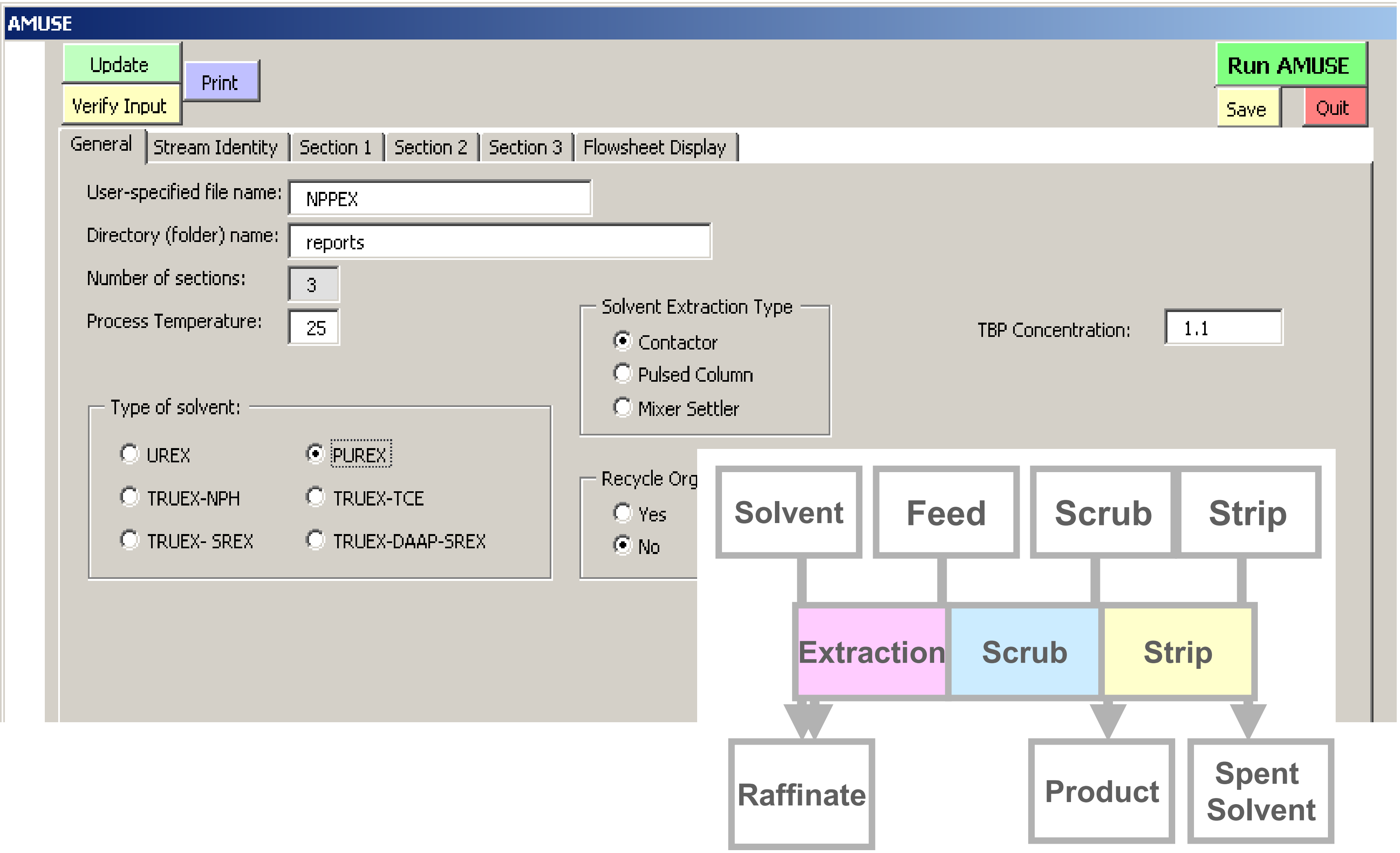
General Input Form



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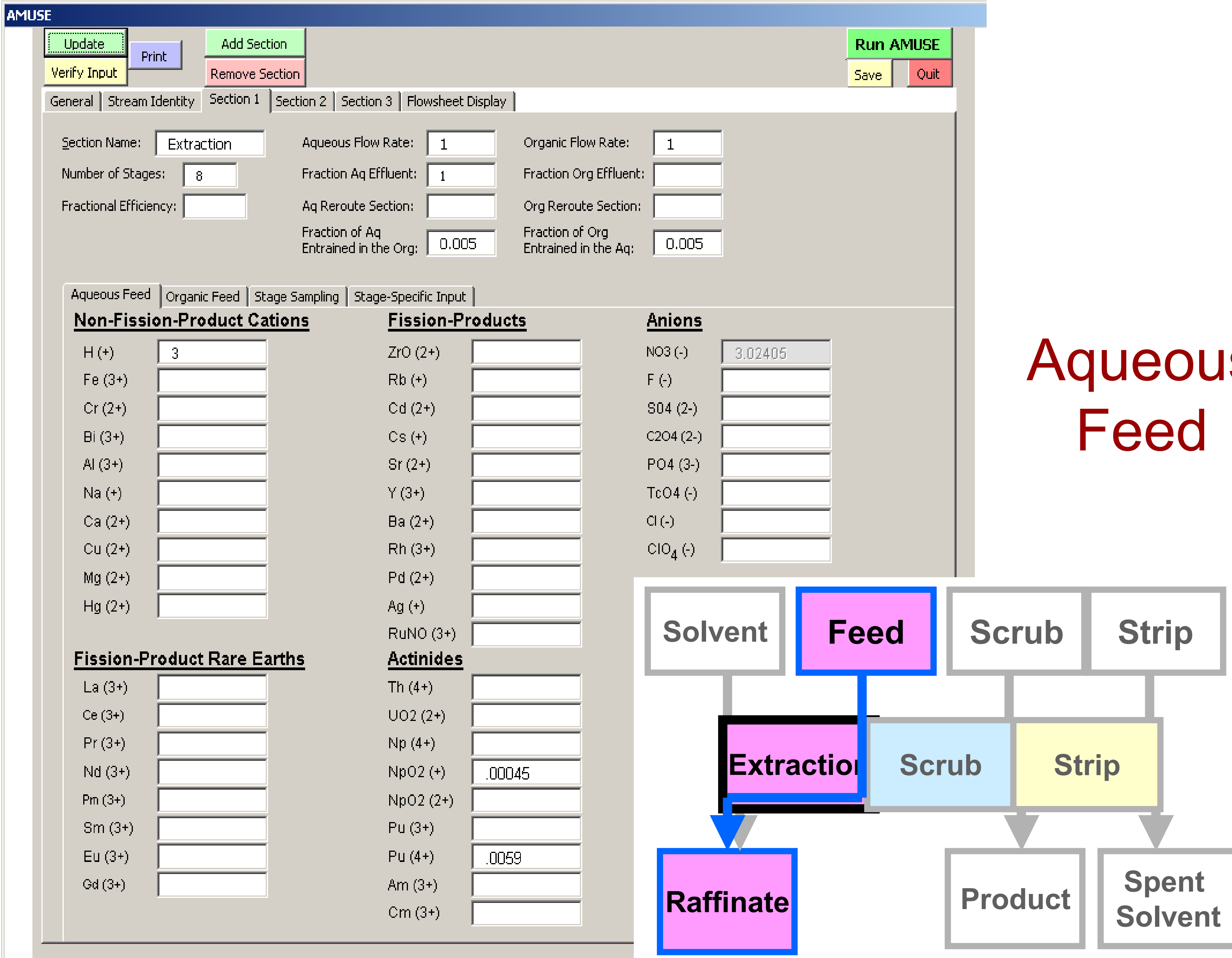
Section Data -- Extraction



Aqueous Feed

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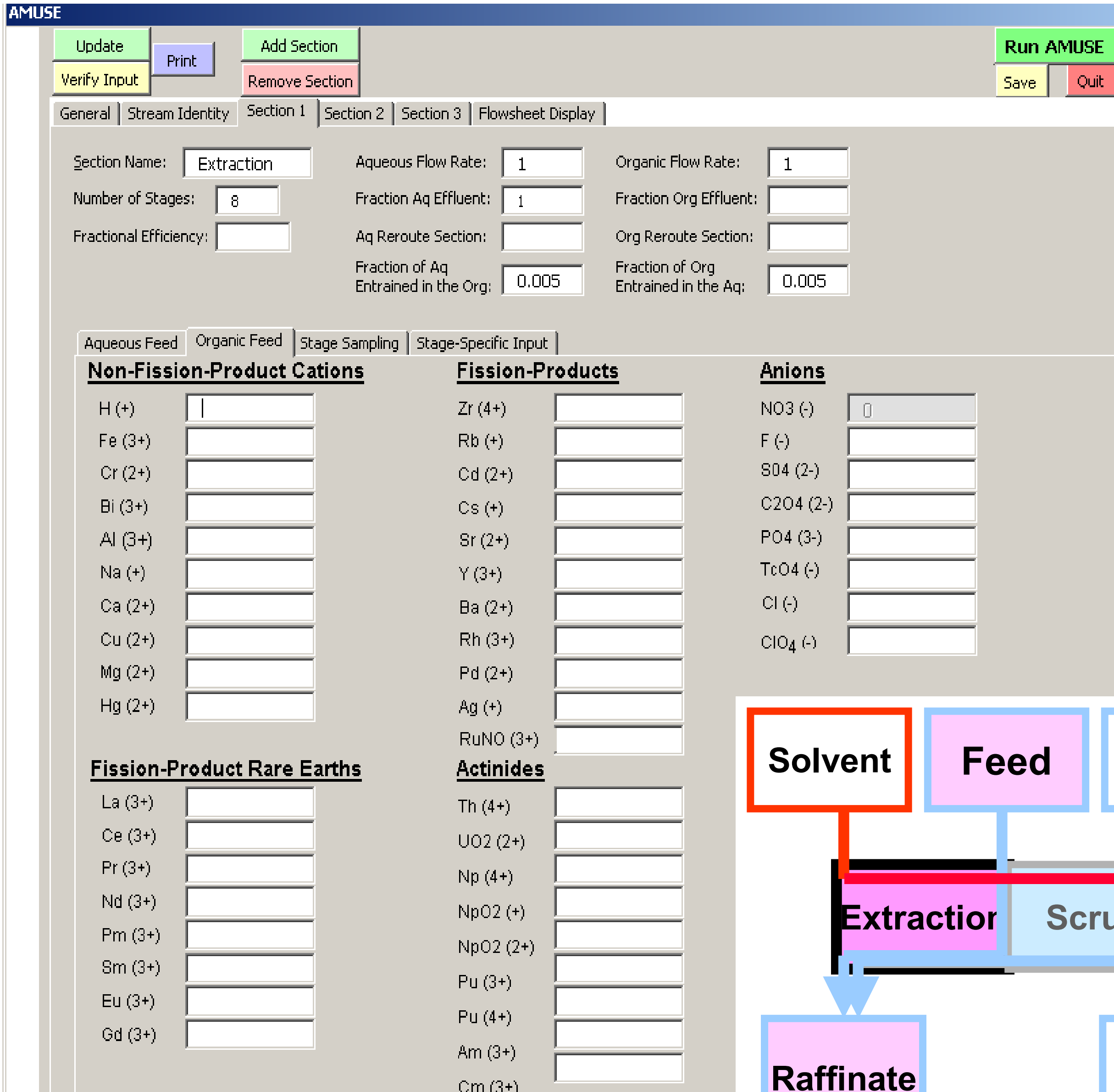
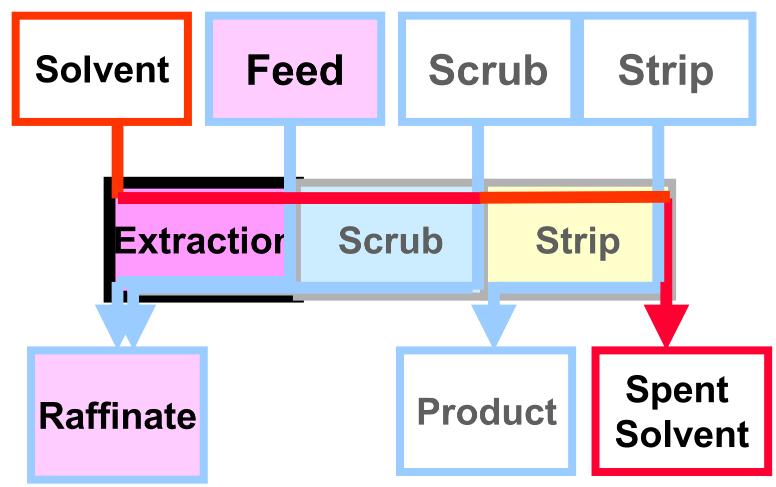
Section Data -- Extraction



Organic Feed



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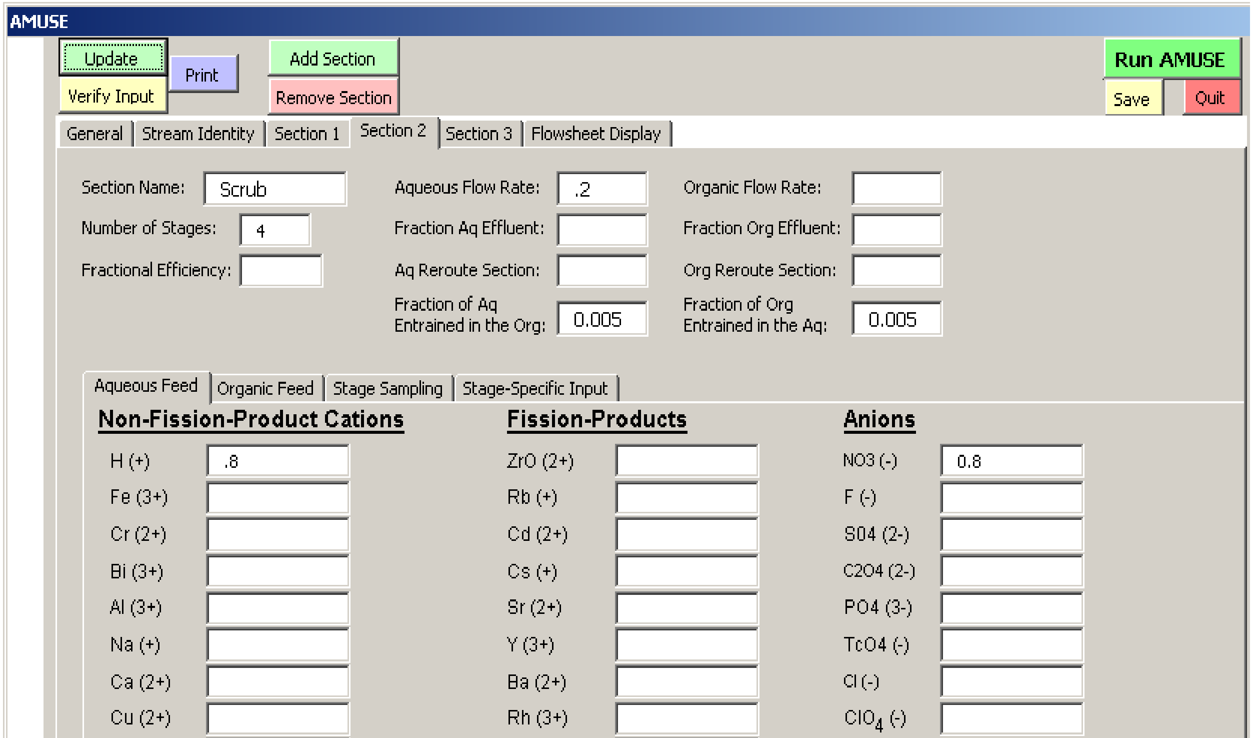
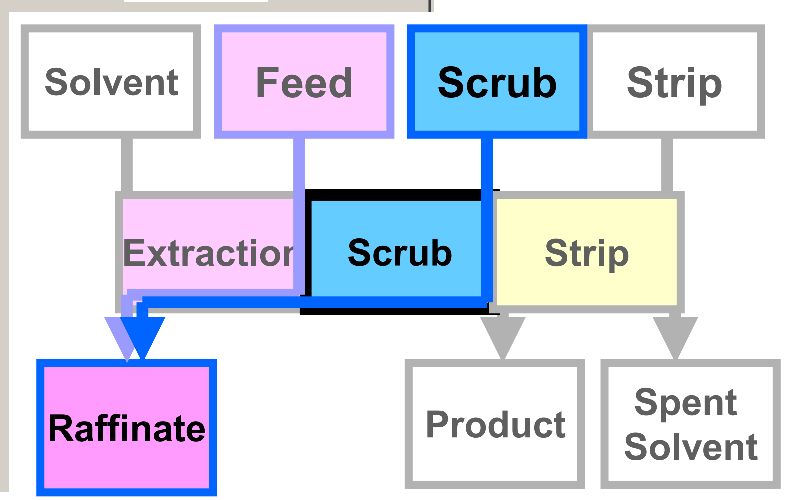
Section Data -- Scrub



Aqueous Feed



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Section Data -- Strip

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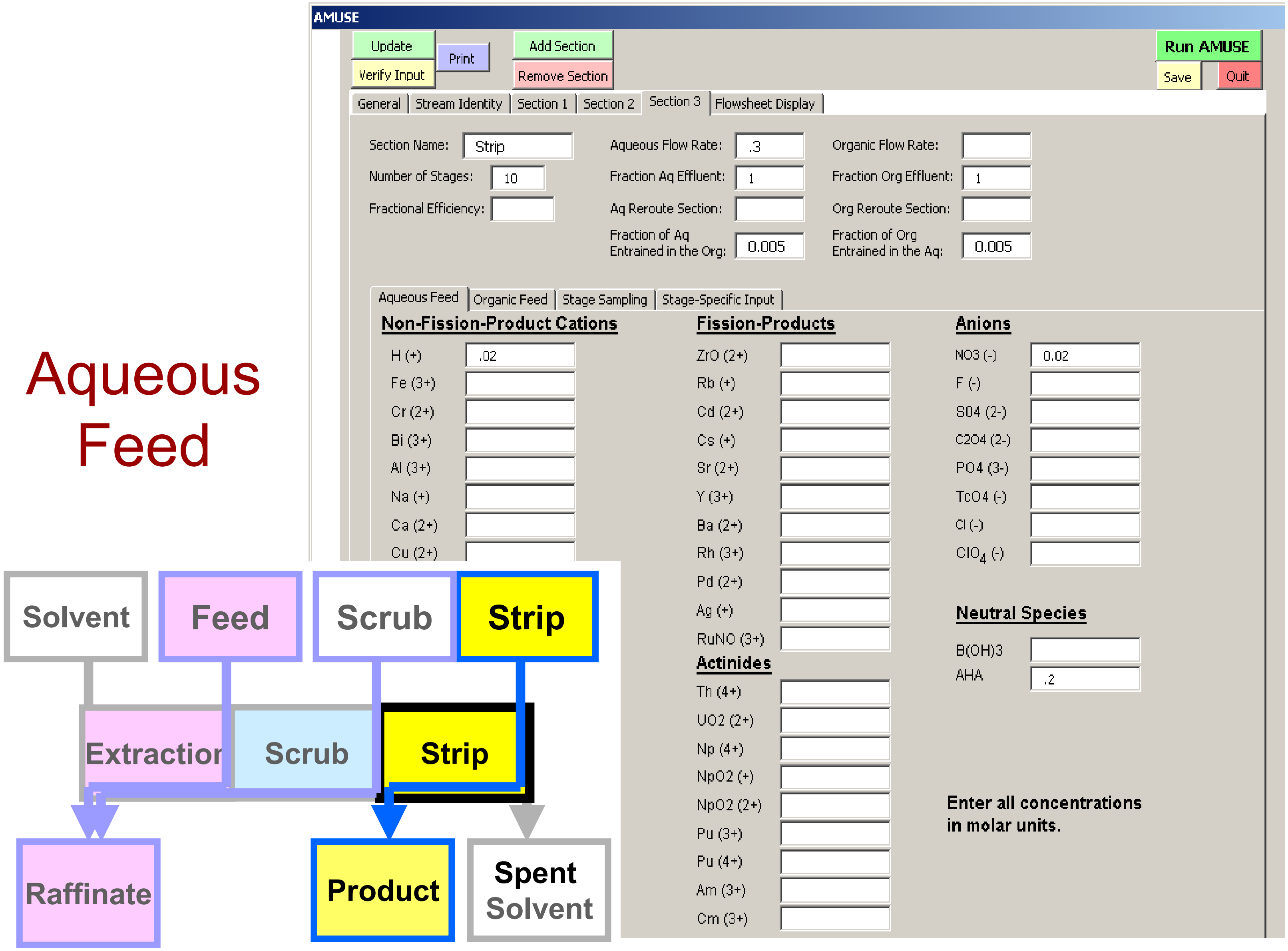
Aqueous Feed



Stage-Specific Input

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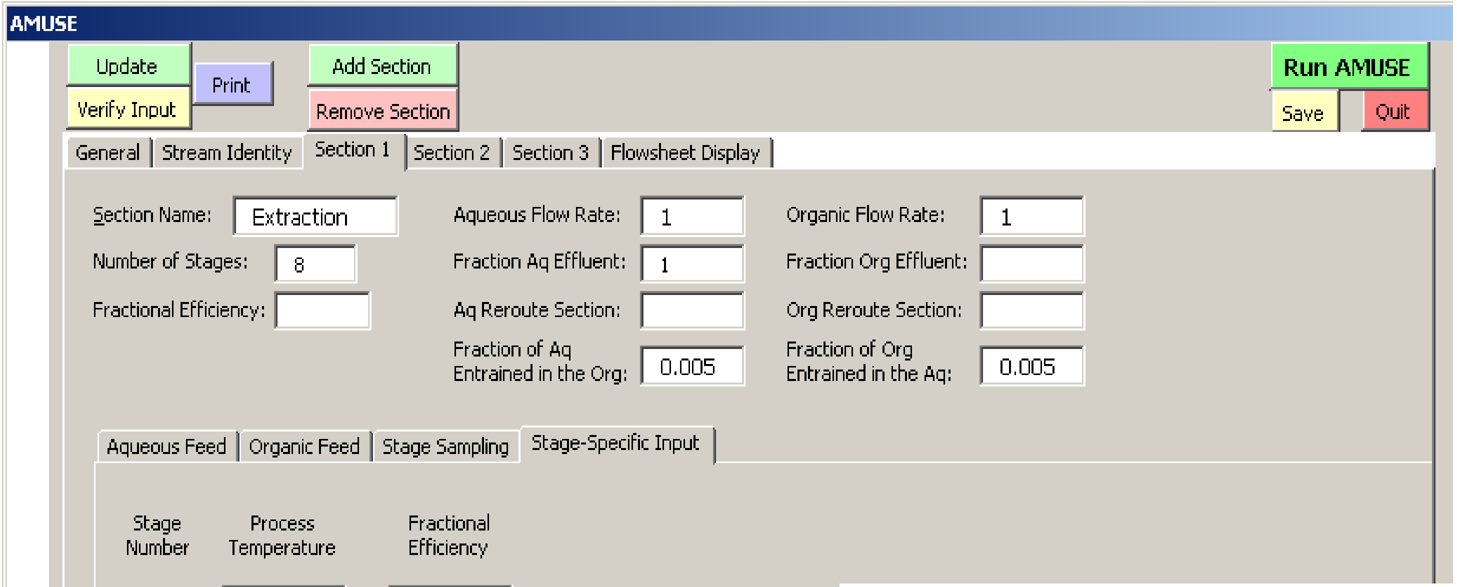
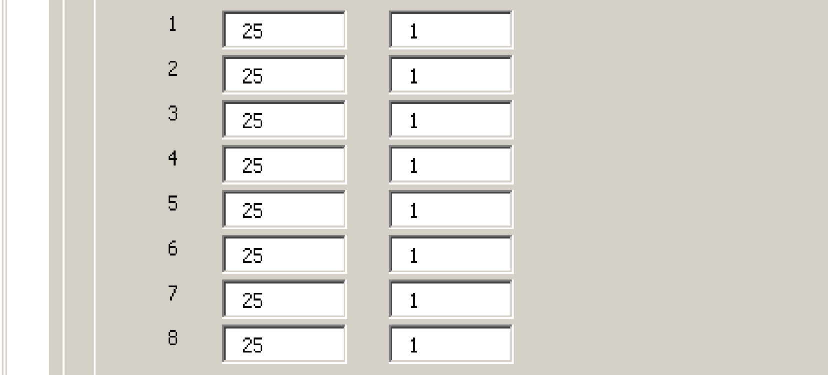
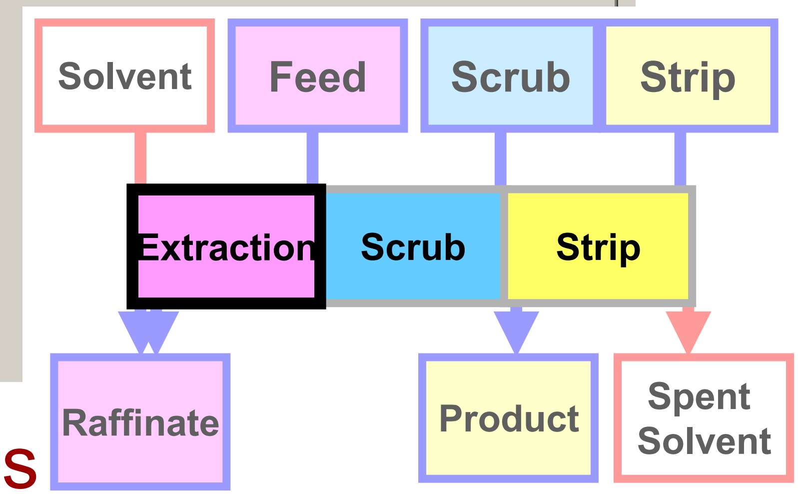






Extraction Section Stages

AMUSE Reports

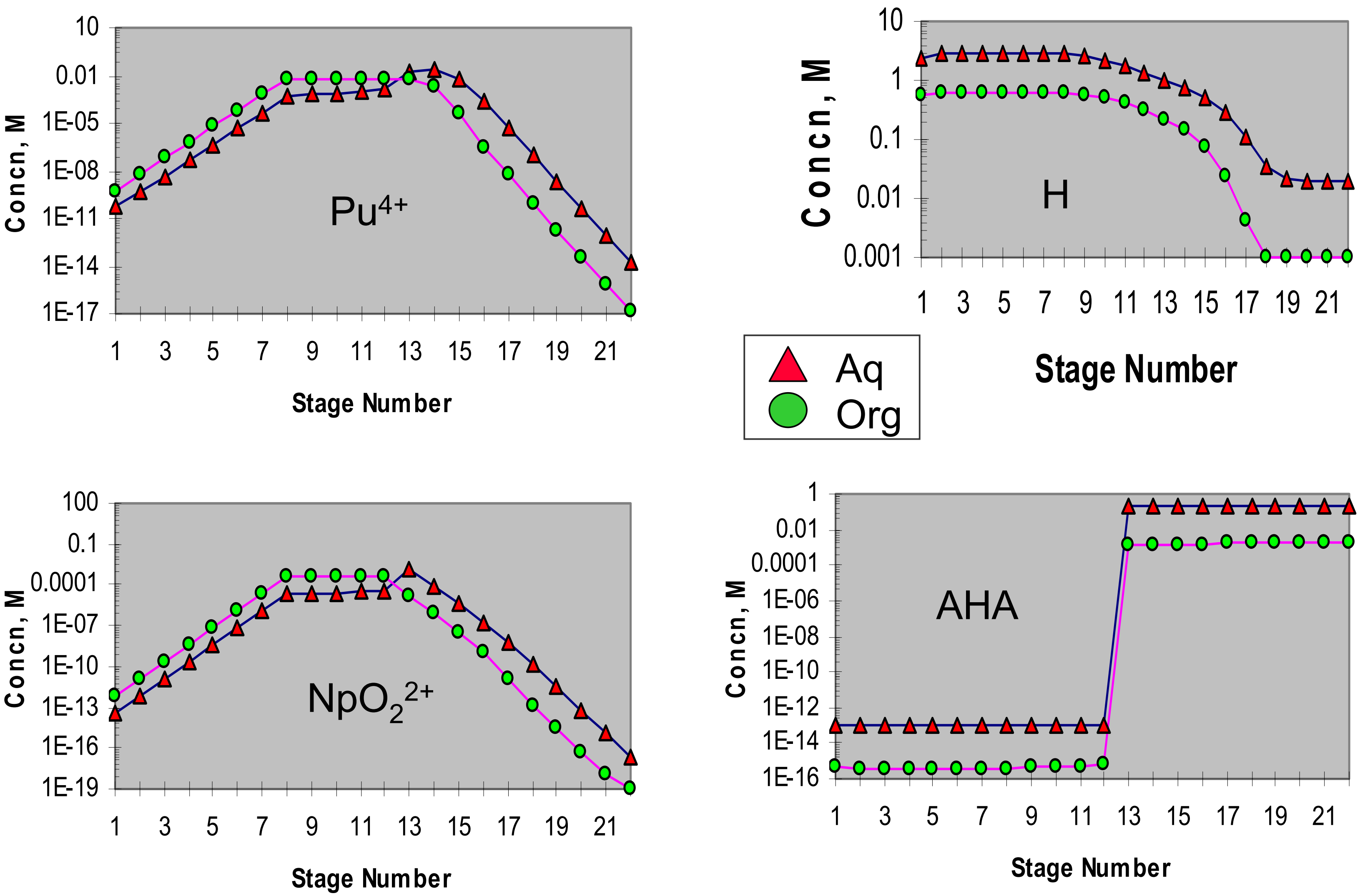
GRAPHICAL

- A figure is created for each component
  - Showing its concentrations in both the organic and aqueous phase of every stage

TABULAR

- Tabular reports are created for
  - Influent and effluent compositions and flow rates
  - Stage profiles that include
    - Distribution ratios
    - Component concentrations in organic and aqueous phases

Graphical Output



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Tabular Output

Section	Name	Stage Number	Phase	Flow Direction	Stream Identity	Flow Rate	Component Concentration, M			
							H	AHA	NpO2_2	Pu_4
1	Extraction	1	O	in	DX	1	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	Extraction	8	A	in	DF	1	3.000E+00	1.000E-13	4.500E-04	5.900E-03
2	scrub	12	A	in	DS	0.2	8.000E-01	1.000E-13	0.000E+00	0.000E+00
3	strip	22	A	in	EF	0.3	2.000E-02	2.000E-01	0.000E+00	0.000E+00
1	Extraction	1	A	out	DW	1.1949749	2.385E+00	9.952E-14	3.829E-14	5.980E-11
3	strip	13	A	out	EW	0.3050266	1.035E+00	1.915E-01	1.475E-03	1.934E-02
3	strip	22	O	out	EP	1	1.926E-04	1.594E-03	2.196E-20	1.506E-17

Component Name	Phase		Stage-to-Stage Profile for each Component						
		Section No.	1	1	1	1	3	3	3
		Stage No.	1	2	3	4	20	21	22
H	Aqueous	x, M	2.385E+00	2.836E+00	2.912E+00	2.923E+00	2.011E-02	2.001E-02	2.000E-02
	Organic	y, M	5.416E-01	6.296E-01	6.435E-01	6.457E-01	1.945E-04	1.927E-04	1.926E-04
		D value	2.271E-01	2.220E-01	2.210E-01	2.209E-01	9.675E-03	9.632E-03	9.629E-03
AHA	Aqueous	x, M	9.952E-14	9.989E-14	9.986E-14	9.985E-14	2.000E-01	2.000E-01	2.000E-01
	Organic	y, M	4.387E-16	4.020E-16	3.964E-16	3.955E-16	1.594E-03	1.594E-03	1.594E-03
		D value	4.408E-03	4.024E-03	3.969E-03	3.961E-03	7.968E-03	7.968E-03	7.968E-03
NpO2_2	Aqueous	x, M	3.829E-14	5.675E-13	9.857E-12	1.769E-10	5.630E-14	1.114E-15	2.196E-17
	Organic	y, M	7.100E-13	1.313E-11	2.365E-10	4.269E-09	5.630E-17	1.114E-18	2.196E-20
		D value	1.854E+01	2.313E+01	2.399E+01	2.413E+01	1.000E-03	1.000E-03	1.000E-03
Pu_4	Aqueous	x, M	5.980E-11	4.870E-10	4.704E-09	4.702E-08	3.862E-11	7.639E-13	1.506E-14
	Organic	y, M	5.450E-10	5.895E-09	5.959E-08	5.998E-07	3.862E-14	7.639E-16	1.506E-17
		D value	9.114E+00	1.210E+01	1.267E+01	1.276E+01	1.000E-03	1.000E-03	1.000E-03

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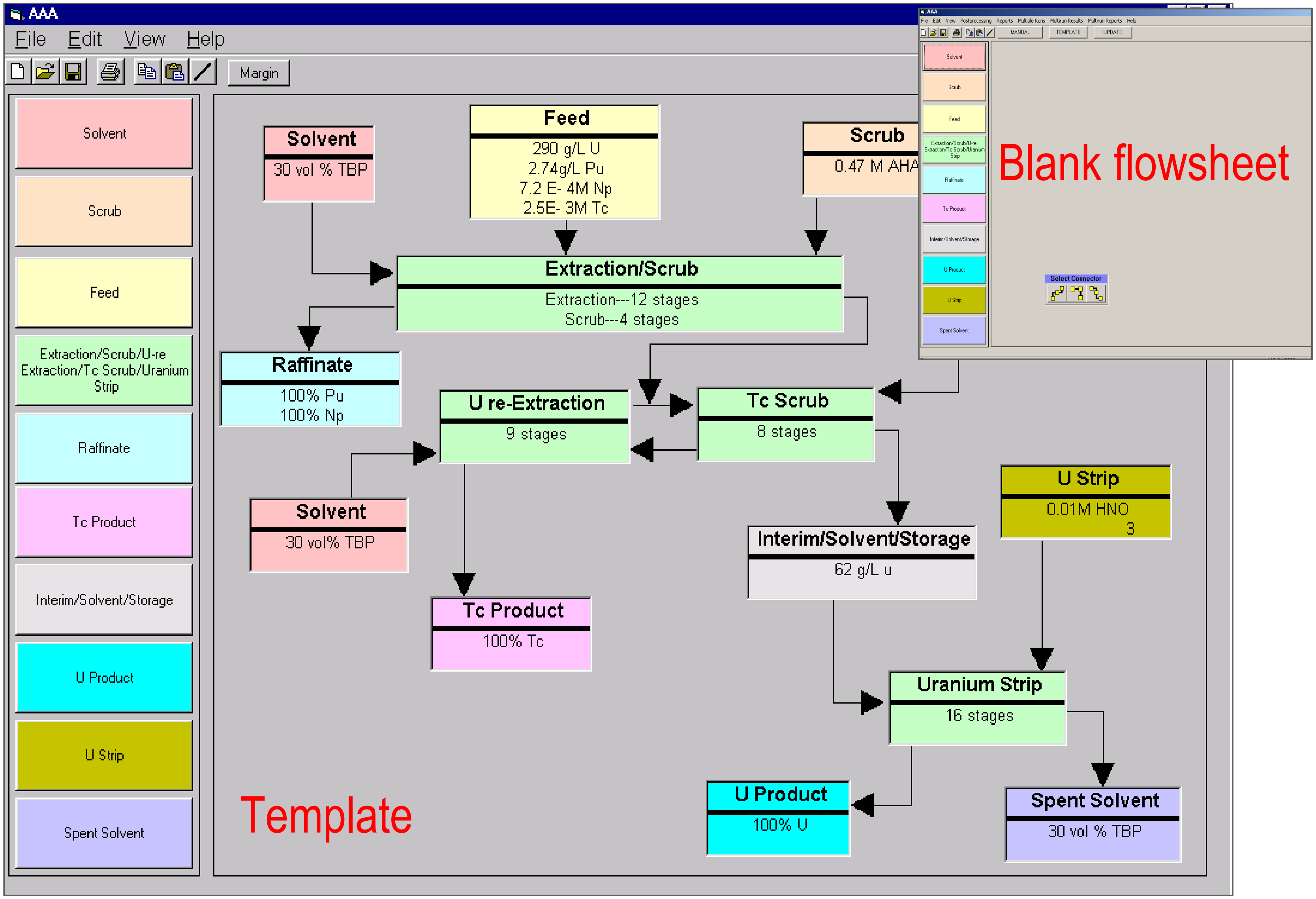
UNLV Partnership

- Working with Nevada Center for Advanced Computational Methods (NCACM)
  - Developing and implementing a graphical user interface (GUI) for AMUSE
  - Designing a systems-engineering model to optimize the UREX+ process

Graphical User Interface



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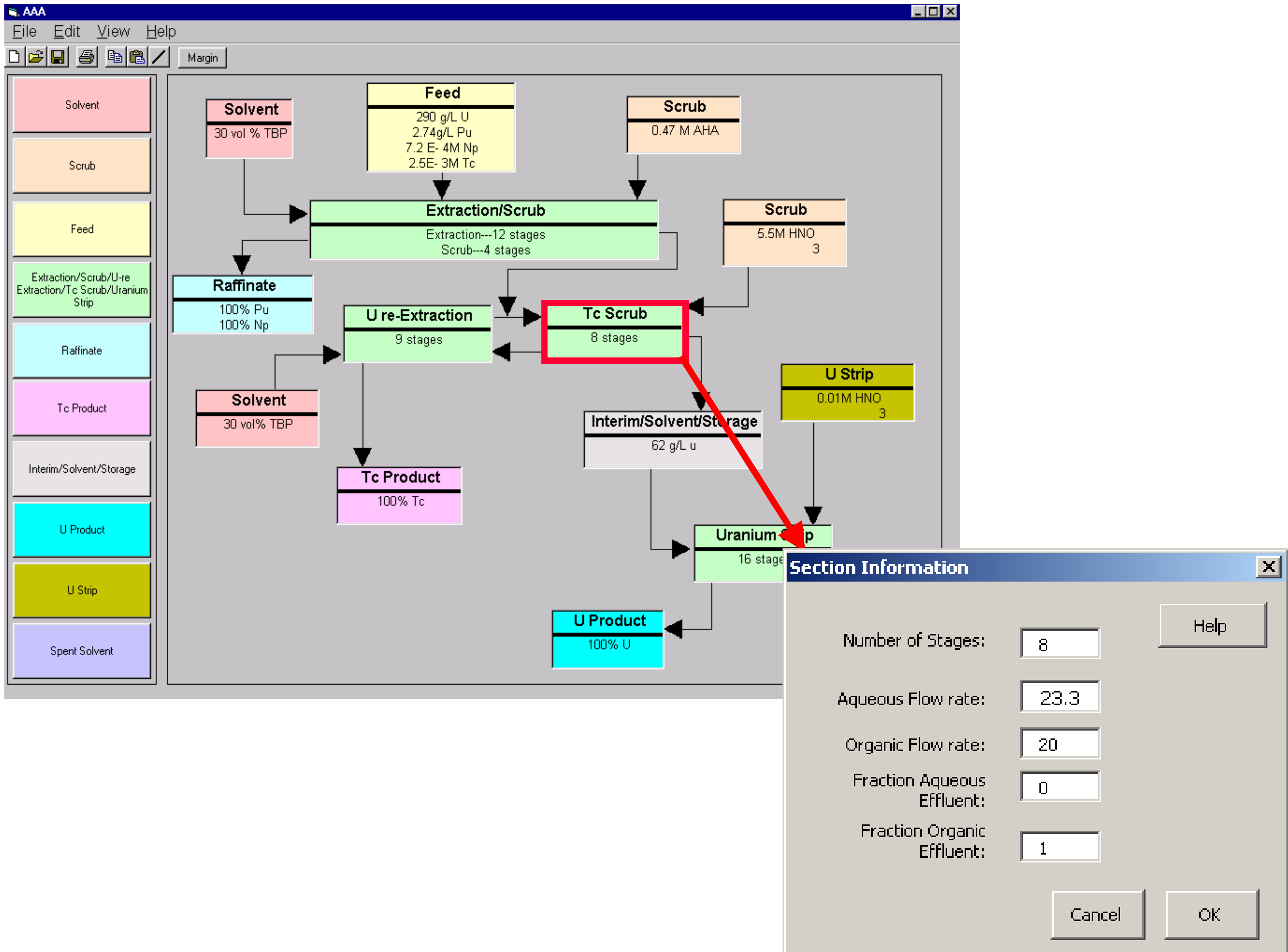
Graphical User Interface



Participants from NCACM

- Faculty
  - Dr. Yitung Chen - Principal Investigator
  - Dr. Randy Clarksean - Co-Principal Investigator
  - Dr. Hsuan-Tsung (Sean) Hsieh – Interface and database design and development
- Graduate Students
  - Lijian Sun – Systems engineering model design
  - Haritha Royyuru – Interface design and implementation

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Conclusion and Future Development

Conclusion

- AMUSE has been an important tool for developing the UREX process and will continue to be for the UREX+ process

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Future Model Development

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- Add all potential UREX+ processes
  - Using literature data
  - Data collected at SRTC, ORNL, INEEL, LANL and ANL
- Improve model predictions based on
  - Demonstration results
  - Fundamental studies in collaboration with MIT
- Develop monitor-and-control parameters for UREX+ process